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nofile l5-


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L2             3 SEA SSS FUL L1 (    10 REACTIONS)


L1               STR
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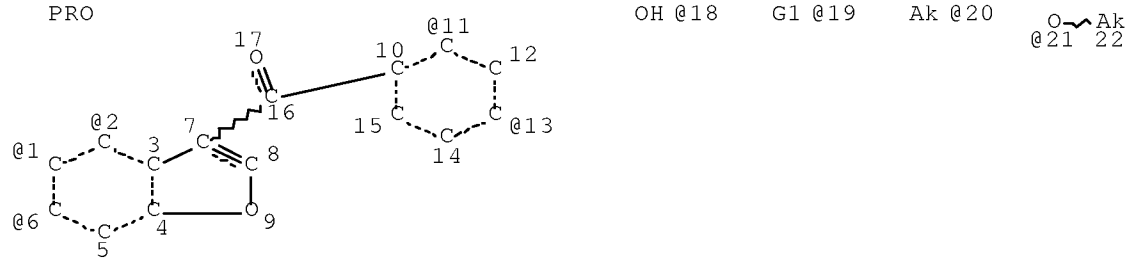


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
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100.0% DONE    2232 VERIFIED      10 HIT RXNS                      3 DOCS
SEARCH TIME: 00.00.02




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                ACT CHANDRAREG/A
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L4            36 SEA SSS FUL L3


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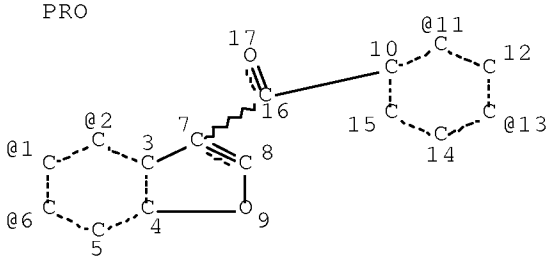
PRO OH @18 G1 @19 Ak @20 O~Ak @21 22



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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L4 36 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 4782 ITERATIONS 36 ANSWERS
SEARCH TIME: 00.00.01

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L6 28 SEA ABB=ON PLU=ON L4/P OR L4 (L) (PREPN/OBI OR PREP/RL)
L7 72233 SEA ABB=ON PLU=ON HALOGEN?/OBI
L8 5521 SEA ABB=ON PLU=ON DEALKY?/OBI
L9 1 SEA ABB=ON PLU=ON L6 AND L8 AND L7
L10 4 SEA ABB=ON PLU=ON L6 AND (L7 OR L8)
L11 81104 SEA ABB=ON PLU=ON ETHER#/OBI (L) (REACT?/OBI OR RACT/RL)
L12 9820 SEA ABB=ON PLU=ON FRIEDEL CRAFT#/OBI
L13 2 SEA ABB=ON PLU=ON L6 AND (L11 OR L12)
L14 5 SEA ABB=ON PLU=ON L13 OR L10
D SCAN TI
L15 53655 SEA ABB=ON PLU=ON ACYLAT?/OBI
L16 3 SEA ABB=ON PLU=ON L15 AND L6
L17 6 SEA ABB=ON PLU=ON L16 OR L14
L18 6 SEA ABB=ON PLU=ON L9 OR L14 OR L16

FILE 'CASREACT, CAPLUS' ENTERED AT 11:39:28 ON 27 DEC 2007
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ANSWERS '1-3' FROM FILE CASREACT
ANSWERS '4-6' FROM FILE CAPLUS
E S SGIYTTEETEN A?/AU
L20 0 SEA ABB=ON PLU=ON SHOUTTEETEN A?/AU
L21 5 SEA ABB=ON PLU=ON BLEGER F?/AU
L22 4 SEA ABB=ON PLU=ON MORDACQ F?/AU
L23 69 SEA ABB=ON PLU=ON PIRON J?/AU

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L25          114 SEA ABB=ON  PLU=ON  (L20 OR L21 OR L22 OR L23 OR L24)
L26            2 SEA ABB=ON  PLU=ON  L25 AND L5
L27            1 SEA ABB=ON  PLU=ON  L26 NOT L19


=> fil casreact caplus
FILE 'CASREACT' ENTERED AT 11:44:25 ON 27 DEC 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CAPLUS' ENTERED AT 11:44:25 ON 27 DEC 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)


=> d que stat l19
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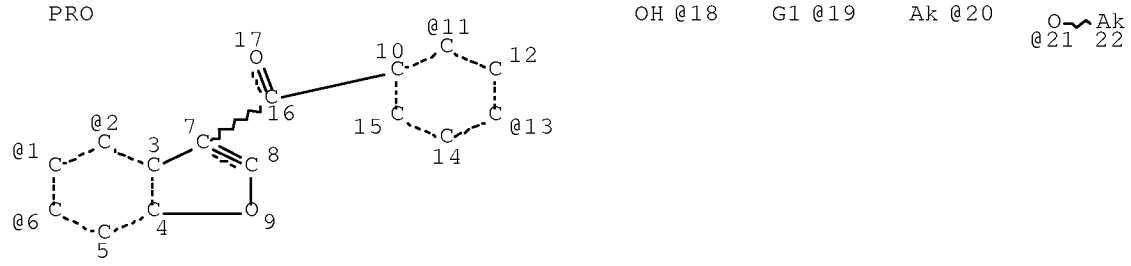


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
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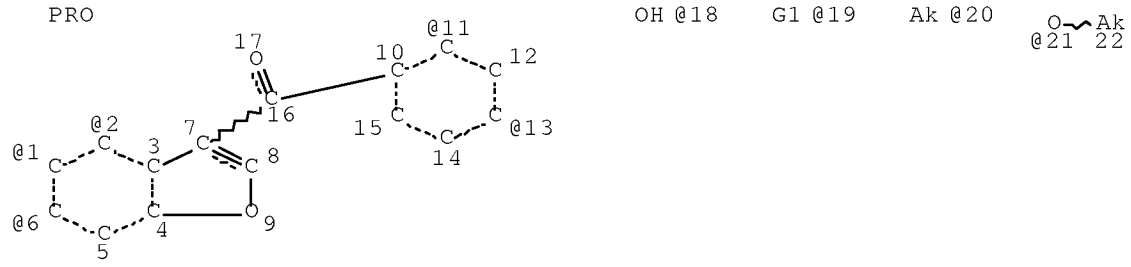


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VPA 19-1/2/6 U
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
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L7         72233 SEA FILE=CAPLUS ABB=ON  PLU=ON  HALOGEN?/OBI
L8          5521 SEA FILE=CAPLUS ABB=ON  PLU=ON  DEALKY?/OBI
L9             1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L6 AND L8 AND L7
L10            4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L6 AND (L7 OR L8)
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L14            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 OR L10
L15        53655 SEA FILE=CAPLUS ABB=ON  PLU=ON  ACYLAT?/OBI
L16            3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 AND L6
L18            6 SEA FILE=CAPLUS ABB=ON  PLU=ON  L9 OR L14 OR L16
L19            6 DUP REM L2 L18 (3 DUPLICATES REMOVED)


=> d que nos l27
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L3               STR
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L6            28 SEA FILE=CAPLUS ABB=ON  PLU=ON  L4/P OR L4 (L) (PREPN/OBI OR
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L7         72233 SEA FILE=CAPLUS ABB=ON  PLU=ON  HALOGEN?/OBI
L8          5521 SEA FILE=CAPLUS ABB=ON  PLU=ON  DEALKY?/OBI
L9             1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L6 AND L8 AND L7
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L12         9820 SEA FILE=CAPLUS ABB=ON  PLU=ON  FRIEDEL CRAFT#/OBI
L13            2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L6 AND (L11 OR L12)
L14            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13 OR L10
L15        53655 SEA FILE=CAPLUS ABB=ON  PLU=ON  ACYLAT?/OBI
L16            3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 AND L6
L18            6 SEA FILE=CAPLUS ABB=ON  PLU=ON  L9 OR L14 OR L16
L19            6 DUP REM L2 L18 (3 DUPLICATES REMOVED)
L20            0 SEA SHOUTTEETEN A?/AU
L21            5 SEA BLEGER F?/AU
L22            4 SEA MORDACQ F?/AU
L23           69 SEA PIRON J?/AU
L24           45 SEA SCHOUTEETEN A?/AU
L25          114 SEA (L20 OR L21 OR L22 OR L23 OR L24)
L26            2 SEA L25 AND L5
L27            1 SEA L26 NOT L19
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L19  ANSWER 1 OF 6  CASREACT  COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER:        144:450603  CASREACT  Full-text
TITLE:                   Process for acylation of (hydroxy)-containing aromatic
                         compounds, particularly benzothiophenes, with aromatic
                         hydroxycarboxylic acids in the presence of Lewis acids
                         and halogenosilanes
INVENTOR(S):             Bourgeois, Damien
PATENT ASSIGNEE(S):      Rhodia Chimie, Fr.
SOURCE:                  Fr. Demande, 35 pp.
                         CODEN: FRXXBL
DOCUMENT TYPE:           Patent
LANGUAGE:                French
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     FR 2877341         A1   20060505       FR 2004-11646    20041102
     CA 2585714         A1   20060511       CA 2005-2585714  20051028
     WO 2006048545      A1   20060511       WO 2005-FR2716   20051028
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     EP 1809617         A1   20070725       EP 2005-815207   20051028
         R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
     IN 2007DN03286     A    20070831       IN 2007-DN3286   20070501
PRIORITY APPLN. INFO.:                      FR 2004-11646    20041102
                                            WO 2005-FR2716   20051028
OTHER SOURCE(S):         MARPAT 144:450603
AB    The invention is related to a process for the acylation of aromatic compds.,
      particularly benzothiophenes I [R4 = alkyl, halogenophenyl, (un)substituted
      Ph; each R5 = independently H , NO2, alkyl, alkoxy, halo, CF3, etc.; n = 0-3],
      with aromatic hydroxycarboxylic acids II [each R7 = H or a substituent,
      especially alkyl, alkoxy, NO2, CN; m < 4], in the presence of a Lewis acid and
      a halogenosilane to give the ketones III.  The advantages include acylation of
      hydroxy-containing substrates and/or agents without OH group protection,
      absence of toxic materials and simple procedure.  Thus, successive addition of
      4-hydroxybenzoic acid, chlorobenzene, methyltrichlorosilane, 2-butyl-5-
      nitrobenzofuran (IV) and FeCl3 at 23°, and stirring at 40° for 5 h gave 2-
      butyl-3-(4- hydroxybenzoyl)-5-nitrobenzofuran in 78% selectivity at 95%
      conversion of IV.



RX(1) OF 1     A  +  B  ===>  C
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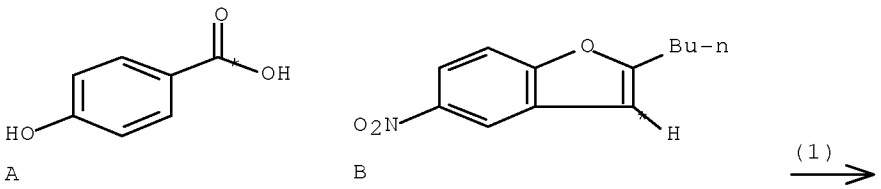
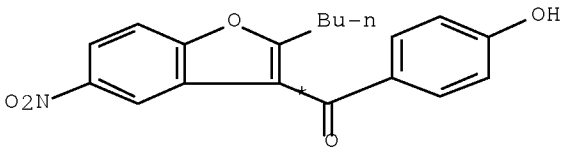




C
YIELD 82%

RX(1) RCT A 99-96-7

STAGE(1)
SOL 108-90-7 PhCl
CON room temperature -> 40 deg C

STAGE(2)
RGT D 7705-08-0 FeCl3, E 75-79-6 MeSiCl3
CON 15 minutes, 40 deg C

STAGE(3)
RCT B 133238-87-6
SOL 108-90-7 PhCl
CON SUBSTAGE(1) 12 minutes, 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
SUBSTAGE(3) 40 deg C -> 30 deg C

STAGE(4)
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 17 minutes, 30 deg C
SUBSTAGE(2) 10 minutes, 30 deg C

PRO C 141645-16-1
NTE optimization study, optmiized on temperature, order and mode of addition of reaction participants

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

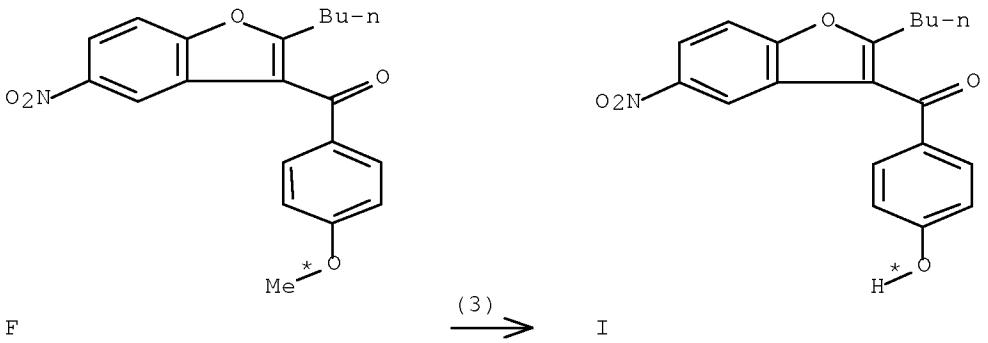
L19 ANSWER 2 OF 6 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 143:97254 CASREACT Full-text
TITLE: Process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and dealkylation
INVENTOR(S): Schouteeten, Alain; Bleger, Francois; Mordacq,

Francoise; Piron, Jerome
PATENT ASSIGNEE(S): Clariant France, Fr.
SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2864536	A1	20050701	FR 2003-15398	20031224
FR 2864536	B1	20060317		
WO 2005066149	A1	20050721	WO 2004-IB4158	20041215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1699772	A1	20060913	EP 2004-801395	20041215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1898226	A	20070117	CN 2004-80038285	20041215
JP 2007517012	T	20070628	JP 2006-546365	20041215
NO 2006002936	A	20060922	NO 2006-2936	20060623
IN 2006CN02324	A	20070706	IN 2006-CN2324	20060626
US 2007155831	A1	20070705	US 2006-584440	20061129
PRIORITY APPLN. INFO.:			FR 2003-15398	20031224
			WO 2004-IB4158	20041215

AB The invention is related to the preparation of benzofurans I [R = linear or branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5- nitrobenzofuran with SOCl2 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlCl3 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°).

RX(3) OF 14 ...F ===> I



F I

RX(3) RCT F 141627-42-1

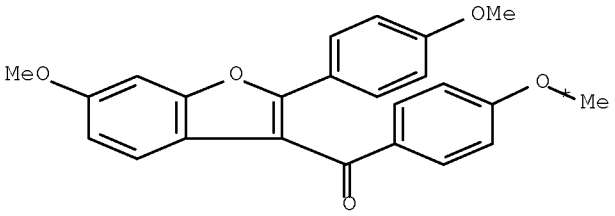
STAGE(1)
RGT H 7446-70-0 AlCl3
SOL 108-90-7 PhCl
CON 7 hours, room temperature -> 60 deg C

STAGE(2)
RGT J 7732-18-5 Water

PRO I 141645-16-1
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 6 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 122:105333 CASREACT Full-text
TITLE: Regioselectivity in the Alkaline Thiolate Deprotection of Aryl Methyl Ethers
AUTHOR(S): Dodge, Jeffrey A.; Stocksdale, Mark G.; Fahey, Kennan J.; Jones, C. David
CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Journal of Organic Chemistry (1995), 60(3), 739-41
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The regioselective deprotection of aryl Me ethers using sodium ethanethiolate in DMF was systematically explored. Electronic factors appear to control the observed selectivity, with Me ethers para to electron-withdrawing groups reacting preferentially with the thiol anion. In addition, substituent effects indicate a relationship between the Hammet constant and the efficacy of the reaction, with more electron-poor species providing higher yields of demethylated product. A variety of these substituents (NO2, CN, acetyl) provide useful yields of deprotected product, thereby adding synthetic utility to this general method.

RX(4) OF 15 I ===> J



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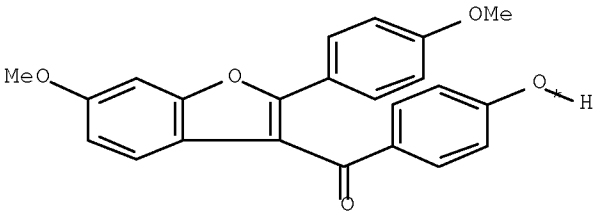

J
YIELD 75%

RX(4) RCT I 160663-54-7
RGT C 811-51-8 NaSEt
PRO J 160663-56-9
SOL 68-12-2 DMF
NTE REGIOSELECTIVE

L19 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:815935 CAPLUS Full-text
DOCUMENT NUMBER: 145:230520
TITLE: Preparation of benzofurans and related derivatives as tubulin polymerization inhibitors for treating neoplasm and inflammation
INVENTOR(S): Chaplin, Jason Hugh; Gill, Gurmit Singh; Grobelny, Damian Wojciech; Flynn, Bernard Luke
PATENT ASSIGNEE(S): Iliad Chemicals Pty Ltd, Australia
SOURCE: PCT Int. Appl., 147pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006084338	A1	20060817	WO 2006-AU192	20060214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,

MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

AU 2006212726	A1	20060817	AU 2006-212726	20060214
CA 2597447	A1	20060817	CA 2006-2597447	20060214
EP 1848704	A1	20071031	EP 2006-704869	20060214

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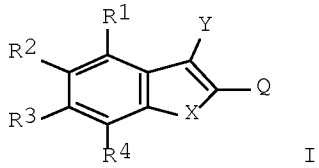
PRIORITY APPLN. INFO.: US 2005-652668P P 20050214
WO 2006-AU192 W 20060214

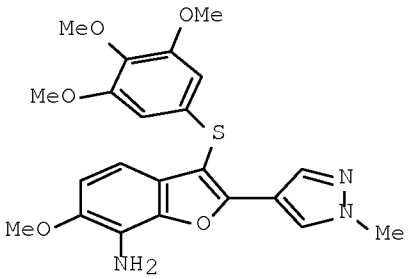
OTHER SOURCE(S): MARPAT 145:230520

ED Entered STN: 17 Aug 2006

GI



I



II

AB Title compds. I [X = O, S, SO, SO2, Se, SeO, SeO2, NH and derivs.; R1-R4 = independently H, CO2H, CN, OH, NO2, (un)substituted acyl, arylalkoxy, aryl, oxyacylamino, etc.; Y = (un)substituted Ph, phenylcarbonyl, phenoxy, phenylsulfanyl, etc.; Q = (un)substituted heteroaryl, heterocyclyl, heteroarylcarbonyl, etc.; with provisos; and their salts] were prepared as tubulin polymerization inhibitors. Thus, Sonogashira coupling of 2,4-dimethoxy-3-nitroiodobenzene (preparation given) with 4-ethynyl-1-methyl-1H-pyrazole, cyclization with bis(pyridine)iodonium tetrafluoroborate, Stille coupling with trimethyl(3,4,5-trimethoxyphenyl)stannane, and reduction with Zn/AcOH gave benzofuran II. II inhibited tubulin polymerization (IC50 = 1.5±0.1 μM). Selected I inhibited proliferation of MCF-7 breast cancer cells and activated HUVEC cells. I are useful for treating neoplasm and inflammation.

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT 905751-61-3P, [2-(1-Benzyl-1H-pyrazol-4-yl)-6-methoxybenzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905751-63-5P, [7-Hydroxy-6-methoxy-2-(1H-pyrazol-4-yl)benzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905751-68-0P, 2-(1-Methylpyrazol-4-yl)-3-(3,4,5-trimethoxybenzoyl)-6-

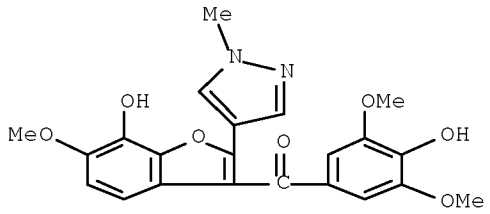
methoxy-7-hydroxybenzofuran 905751-70-4P, 2-(1-Methylpyrazol-4-yl)-3-(3,5-dimethoxybenzoyl)-6-methoxy-7-hydroxybenzofuran 905751-75-9P 905751-76-0P, 2-[4-[6-Methoxy-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan-2-yl]pyrazol-1-yl]acetamide 905751-77-1P, [6-Methoxy-2-[1-(4-methoxyphenyl)-1H-pyrazol-4-yl]benzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905751-78-2P, [2-[1-(2-Dimethylaminoethyl)-1H-pyrazol-4-yl]-6-methoxybenzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905751-79-3P, 2-[4-[7-Hydroxy-6-methoxy-3-(3,4,5-trimethoxybenzoyl)benzofuran-2-yl]pyrazol-1-yl]acetamide 905751-81-7P, [2-(1-Methyl-1H-Imidazol-4-yl)-6-methoxybenzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905751-82-8P 905751-85-1P 905751-88-4P 905751-91-9P 905751-95-3P 905751-97-5P, (2S)-2-Amino-3-hydroxy-N-[6-methoxy-2-(1-methyl-1H-pyrazol-4-yl)-3-(3,4,5-trimethoxybenzoyl)benzofuran-7-yl]propanamide Hydrochloride 905752-01-4P 905752-03-6P, [6-Methoxy-2-(1-methyl-1H-pyrazol-4-yl)-1H-indol-3-yl](3,4,5-trimethoxyphenyl)methanone 905752-09-2P, [6-Methoxy-7-nitro-2-(1-methyl-1H-pyrazol-4-yl)benzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905752-10-5P, 7-Amino-6-methoxy-2-(1-methyl-1H-pyrazol-4-yl)-3-[(3,4,5-trimethoxyphenyl)thio]benzo[b]furan 905752-12-7P, [7-Fluoro-6-methoxy-2-(1-methyl-1H-pyrazol-4-yl)benzofuran-3-yl](3,4,5-trimethoxyphenyl)methanone 905752-16-1P, 2-[4-[7-Fluoro-6-methoxy-3-(3,4,5-trimethoxybenzoyl)benzofuran-2-yl]-1H-pyrazol-1-yl]acetamide 905752-18-3P 905752-22-9P 905752-40-1P, 2-(6-Methoxypyridin-3-yl)-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzofuran 905752-42-3P, 2-(Thiophen-3-yl)-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-43-4P, 2-(3,5-Dimethylisoxazol-4-yl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-44-5P, 2-(1-Isobutylpyrazol-4-yl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-45-6P, 2-[5-(Formyl)thiophen-2-yl]-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-46-7P, 2-(1-Imidazolyl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-47-8P, 2-(1,2,3-Triazol-1-yl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-48-9P, 2-(1-Pyrazolyl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-49-0P, 2-(1,2,4-Triazol-1-yl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-50-3P, 2-(1-Pyrrolyl)-7-hydroxy-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-51-4P, 2-(4-Methylpiperazino)-3-(3,4,5-trimethoxybenzoyl)-6-methoxybenzo[b]furan 905752-52-5P, 2-(2-Furyl)-6-methoxy-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan 905752-54-7P, 7-Hydroxy-6-methoxy-2-(2H-tetrazol-5-yl)-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan 905752-56-9P, 7-Hydroxy-6-methoxy-2-(2H-[1,2,3]triazol-4-yl)-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan 905752-58-1P 905752-59-2P 905752-62-7P, [4-[6-Methoxy-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan-2-yl]pyrazol-1-yl]acetic acid 905752-63-8P, (2S)-2-Amino-3-hydroxy-N-[6-methoxy-2-(1-methyl-1H-pyrazol-4-yl)-3-(3,4,5-trimethoxybenzoyl)benzofuran-7-yl]propanamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzofurans and related derivs. as tubulin polymerization inhibitors for treating neoplasm and inflammation)

IT 4371-79-3, Carbon diiodide 7726-95-6, Bromine, reactions 7789-33-5, Iodine bromide (IBr)
RL: RCT (Reactant); RGT (Reagent); RACT (Reactant or reagent)
(halogenation agent; preparation of benzofurans and related derivs. as tubulin polymerization inhibitors for treating neoplasm and inflammation)

IT 905752-18-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation);
USES (Uses)
(drug candidate; preparation of benzofurans and related derivs. as tubulin polymerization inhibitors for treating neoplasm and inflammation)

RN 905752-18-3 CAPLUS
CN Methanone, (4-hydroxy-3,5-dimethoxyphenyl)[7-hydroxy-6-methoxy-2-(1-methyl-1H-pyrazol-4-yl)-3-benzofuranyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1329213 CAPLUS Full-text
DOCUMENT NUMBER: 144:51437
TITLE: Xanthine oxidase inhibitor, 6-hydroxybenzobromarone, and process for the preparation thereof
INVENTOR(S): Endou, Hitoshi; Oikawa, Toshihiro
PATENT ASSIGNEE(S): Torii Pharmaceutical Co., Ltd., Japan; Human Cell Systems, Inc.
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005121112	A1	20051222	WO 2005-JP10671	20050610
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1767531	A1	20070328	EP 2005-748953	20050610
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US 2007185195	A1	20070809	US 2006-628918	20061206
PRIORITY APPLN. INFO.:			JP 2004-172456 A	20040610
			WO 2005-JP10671 W	20050610

ED Entered STN: 22 Dec 2005

AB Process for the preparation of 6-hydroxybenzobromarone (I) was provided. Thus, 2-ethyl-3-(p-hydroxybenzoyl)-6-methoxybenzofuran (6.75 mmol) was reacted with NBS (67.5 mmol) in CH2Cl2 at room temperature for 15 h to give 6-methoxybenzobromarone in 55% yield. Treatment of 6- methoxybenzobromarone (3.74 mmol) with AlCl3 (17.6 mmol) and ethanethiol (7 mL) in CH2Cl2 (35 mL) at ice-bath temperature for 10 min followed by acid work-up and silica gel purification afforded 6-hydroxybenzobromarone in 63% yield. In xanthine oxidase inhibition assays, the IC50 value of compound I was 68 μM. Compound I is claimed useful for the treatment of hyperuricemia, gout, etc.

IC ICM C07D307-80
ICS A61K031-343; A61P013-02; A61P019-02; A61P019-06; A61P043-00

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT Dealkylation
(preparation of 6-hydroxybenzobromarone via deprotection of 6-methoxybenzobromarone)

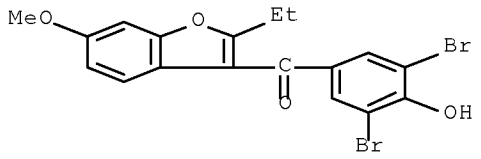
IT 871493-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bromination of 2-ethyl-3-(p-hydroxybenzoyl)-6-methoxybenzofuran using N-bromosuccinimide)

IT 871493-07-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(demethylation of 3-(p-anisoyl)-2-ethyl-6-methoxybenzpfuran using ethanethol sodium salt)

IT 871493-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bromination of 2-ethyl-3-(p-hydroxybenzoyl)-6-methoxybenzofuran using N-bromosuccinimide)

RN 871493-08-2 CAPLUS

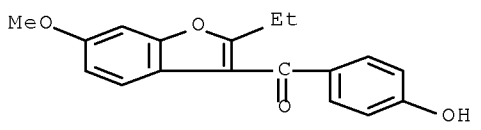
CN Methanone, (3,5-dibromo-4-hydroxyphenyl)(2-ethyl-6-methoxy-3-benzofuranyl)- (CA INDEX NAME)



IT 871493-07-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(demethylation of 3-(p-anisoyl)-2-ethyl-6-methoxybenzpfuran using ethanethol sodium salt)

RN 871493-07-1 CAPLUS

CN Methanone, (2-ethyl-6-methoxy-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:76079 CAPLUS Full-text
DOCUMENT NUMBER: 55:76079
ORIGINAL REFERENCE NO.: 55:14420e-i,14421a-e
TITLE: Study of benzofuran. V. Structure of the diketones obtained from the acylation of 2-ethyl-3-acylbenzofurans
AUTHOR(S): Bisagni, Emile; Royer, Rene
CORPORATE SOURCE: Inst. radium, Paris
SOURCE: Bulletin de la Societe Chimique de France (1960) 1968-76
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB cf. CA 54, 24632a; 55, 505b. 2-Ethyl-3-benzoyl- and 2-ethyl-3-anisoylbenzofurans have been acetylated under Friedel-Crafts conditions with excess AlCl3. Substitution occurred first at the 6-position, next at the 5-position. 2-Acylbenzofurans were not acetylated under the same conditions. To a solution of 1 mole 2-ethyl-3-benzoylbenzofuran (I) and 2 moles AcCl in 700 cc. CS2 was gradually added 2.5 moles AlCl3. The mixture was kept 24 hrs., then decomposed and purified to yield 4.5% I and a mixture, b. 240-60°, which on fractional crystallization from EtOH gave 40% 2-ethyl-3-benzoyl-6-acetylbenzofuran (II), m. 118.5° and 28% 2-ethyl-3-benzoyl-5-acetylbenzofuran (III), m. 68° (ligroine). Similarly, 2-ethyl-3-(4-methoxybenzoyl)benzofuran (IV) with AcCl gave 45% 2-ethyl-3-(4-methoxybenzoyl)-6-acetylbenzofuran (V), m. 118.5-19°, and 7% 2-ethyl-3-(4-methoxybenzoyl)-5-acetylbenzofuran (VI), m. 100-1° (EtOH, then ligroine-C6H6). V was demethylated by refluxing 20 min. with pyridine-HCl to 2-ethyl-3-(4-hydroxybenzoyl)-6- acetylbenzofuran, m. 214-15° (EtOH, or C6H6-ligroine). VI did not respond to similar treatment. NaOH degradation of II gave 4,2-Ac(HO)C6H3CH2COPh (VII), m. 212-13°, BzOH, and 4,2-Ac(HO)C6H3CH2COEt (VIII). Treatment of III with NaOH gave BzOH, 5,2-Ac(HO)C6H3CH2COPh (IX), m. 179°, and 5,2-Ac(HO)C6H3CH2COEt (X). Similarly, V with NaOH gave 4,2-Ac(HO)C6H3CH2COC6H4OMe-p (XI), m. 211°, anisic acid, and VIII. NaOH degradation of VI yielded 5,2-Ac(HO)C6H3CH2COC6H4OMe-p (XII), m. 165-7°, anisic acid, and X. The mixture of VII and VIII obtained from the NaOH degradation of II was methylated with MeI to yield 31% 4,2-Ac(MeO)C6H3CH2COEt (XIII), b17 201-4°, n22 1.5390, and 25.5% 4,2-Ac(MeO)C6H3CH2COPh (XIV), b17 247-8°, m. 66° (ligroine). Methylation of the mixture of VIII and XI gave 11% XIII and 51.1% 4,2-Ac(MeO)C6H3CH2COC6H4OMe-p (XV), b16 275-8°, m. 69-70° (ligroine-20% cyclohexane). Heating VIII in EtOH saturated with HCl gave 90% 2-ethyl-6-acetylbenzofuran (XVI), b12 163-5°, n20.5 1.5845, m. 20-2°; oxime m. 93.5° (dilute Et2O or ligroine). NaOBr treatment of XVI gave 33% 2-ethyl-6-benzofurancarboxylic acid, m. 171-2°. XVI was reduced by N2H4 in (CH2OH)2 to 2,6-diethylbenzofuran, b15 126.5°, n22.5 1.5415. In the same way, VII, heated in EtOH saturated with HCl gave 2-phenyl-6- acetylbenzofuran, m. 103-4° which was reduced by N2H4 to 2-phenyl-6-ethylbenzofuran, m. 52-3° (EtOH). XI heated in EtOH saturated with HCl gave 80% 2-(4-methoxyphenyl)-6-acetylbenzofuran, m. 147° (EtOH-C6H6), which was demethylated to 2-(4-hydroxyphenyl)-6-acetylbenzofuran, m. 228° (EtOH or C6H6) and reduced by N2H4 to 2-(4-hydroxyphenyl)-6-ethylbenzofuran, m. 170-1° (dilute EtOH), b14 244-7°. X heated in EtOH saturated with HCl gave 2-ethyl-5- acetylbenzofuran, b23 179-80°, m. 44-5°; oxime m. 83°. The latter, treated with NaOBr gave 2-ethyl-5-benzofurancarboxylic acid, m. 165° (dilute EtOH). Cyclization of IX yielded 2-phenyl-5-acetylbenzofuran, m. 160° (EtOH), which was reduced by N2H4 in

(CH2OH)2 to 2-phenyl-5-ethylbenzofuran, m. 76° (EtOH), b22 212-14°. XII was also cyclized (EtOH-HCl) to give 68% 2-(4-methoxyphenyl)-5-acetylbenzofuran, m. 170° (EtOH-C6H6), which was simultaneously reduced and demethylated by N2H4 to 2-(4-hydroxyphenyl)-5-ethylbenzofuran, m. 186° (dilute EtOH or C6H6). 5-Ethylsalicylaldehyde, b16 115-16°, n21.5 1.5545, was treated with ClCH2-COMe and KOH in EtOH to yield 57% 2-acetyl-5-ethylbenzofuran, b15 163-4°, m. 33-4° (EtOH), which was reduced to 2,5-diethylbenzofuran (XVII), b14 122-4°, n18 1.5430. XVII was benzoylated (ClCOPh, SnCl4, C6H6) in 67% yield to give 2,5-diethyl-3-benzoylbenzofuran (XVIII), b13 220-2°, n20 1.5995. Anisoylation of XVII gave 2,5-diethyl-3-(4-methoxybenzoyl)benzofuran (XIX), b12 247°, m. 32-3° (EtOH). The latter was demethylated to 2,5-diethyl-3-(4-hydroxybenzoyl)benzofuran, b4 272-3°, m. 135-6° (C6H6). NaOH degradation of XVIII followed by HCl-EtOH recyclization gave 43% PhCO2H, 22.5% XVII, and 40% 2-phenyl-5-ethylbenzofuran. Similar treatment of XIX gave 29.5% anisic acid, 2-(4-methoxyphenyl)-5-ethylbenzofuran, m. 135°, 5,2-Et(HO)C6H3CH2COC6H4OMe-p, m. 118°. Starting with 3-ethylsalicylaldehyde, b28 117-18°, a similar series of reactions was carried out giving 2-acetyl-7-ethylbenzofuran, b19 159-61°, m. 54.5° (EtOH), 2,7-diethylbenzofuran (XX), b20 124-5°, n22 1.5410, and 2,7-diethyl-3-benzoylbenzofuran, b15 228-31°, n21.5 1.6038. NaOH degradation of the latter gave BzOH, XX, and 2-phenyl-7-ethylbenzofuran, b20 220-3°, n24 1.6210.

CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT Acylation
(of 3-acyl-2-ethylbenzofurans, structure of diketones from)

IT Ketones
(structure of di-, from acylation of 3-acyl-2-ethylbenzofurans)

IT 3131-63-3, Benzofuran, 2-ethyl-
(3-acyl derivs., diketones from acylation of)

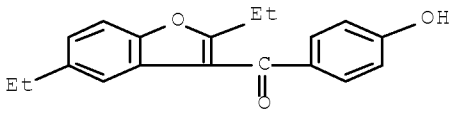
IT 5896-26-4P, Ketone, 2-ethyl-6-benzofuranyl methyl 5896-49-1P, Benzofuran, 2,6-diethyl- 27408-42-0P, Ketone, 2-ethyl-6-benzofuranyl methyl, oxime 28089-83-0P, Ketone, methyl 2-phenyl-6-benzofuranyl 59664-03-8P, Ketone, 7-ethyl-2-benzofuranyl methyl 91495-47-5P, Benzofuran, 2,5-diethyl- 93021-68-2P, Benzofuran, 5-ethyl-2-phenyl- 94066-54-3P, 2,4'''-Biacetophenone, 3'''-hydroxy- 94302-86-0P, Ketone, 2,5-diethyl-3-benzofuranyl p-hydroxyphenyl 95485-40-8P, Ketone, 2-ethyl-5-benzofuranyl methyl 100612-37-1P, Acetophenone, 3'-methoxy-4'-(2-oxobutyl)- 101278-17-5P, Ketone, 2-(p-hydroxyphenyl)-6-benzofuranyl methyl 101594-95-0P, Acetophenone, 2-(5-ethyl-2-hydroxyphenyl)-4'-methoxy- 101596-59-2P, Benzofuran, 5-ethyl-2-(p-methoxyphenyl)- 101894-27-3P, Benzofuran, 6-acetyl-2-ethyl-3-p-hydroxybenzoyl- 101894-27-3P, Phenol, p-(6-acetyl-2-ethyl-3-benzofuranylcarbonyl)- 102158-98-5P, Ketone, 2,5-diethyl-3-benzofuranyl p-methoxyphenyl 103152-25-6P, 2,4'''-Biacetophenone, 3'''-methoxy- 103988-06-3P, 5-Benzofurancarboxylic acid, 2-ethyl- 105207-89-4P, Acetophenone, 4'-hydroxy-3'-(2-oxobutyl)- 105208-20-6P, Acetophenone, 3'-hydroxy-4'-(2-oxobutyl)- 105909-84-0P, Ketone, 2-ethyl-5-benzofuranyl methyl, oxime 106989-39-3P, Ketone, 5-ethyl-2-benzofuranyl methyl 108838-38-6P, 2,3'''-Biacetophenone, 4'''-hydroxy- 108840-63-7P, Benzofuran, 6-ethyl-2-phenyl- 108840-64-8P, Benzofuran, 7-ethyl-2-phenyl- 108840-82-0P, Phenol, p-6-ethyl-2-benzofuranyl- 108842-68-8P, Phenol, p-5-ethyl-2-benzofuranyl- 108980-53-6P, Ketone, 2-(p-methoxyphenyl)-6-benzofuranyl methyl 108983-46-6P, Ketone, 2-(p-methoxyphenyl)-5-benzofuranyl methyl 109155-31-9P, 2,4'''-Biacetophenone, 3'''-hydroxy-4'-methoxy- 109156-66-3P, 2,3'''-Biacetophenone, 4'''-hydroxy-3'-methoxy- 109395-02-0P, 2,4'''-Biacetophenone, 3''',4'-dimethoxy- 109614-26-8P, Benzofuran, 6-acetyl-3-benzoyl-2-ethyl- 109614-90-6P, Benzofuran, 5-acetyl-3-benzoyl-2-ethyl- 109688-24-6P, Ketone, 2,7-diethyl-3-

benzofuranyl phenyl 109690-79-1P, Ketone, 2,5-diethyl-3-benzofuranyl phenyl 109893-46-1P, 1-Propanone, 1-[5(or 6)-acetyl-2-ethyl-3-benzofuranyl]- 109936-61-0P, Benzofuran, 6-acetyl-3-p-anisoyl-2-ethyl- 109938-44-5P, Benzofuran, 5-acetyl-3-p-anisoyl-2-ethyl- 121045-41-8P, Ketone, methyl 2-phenyl-5-benzofuranyl 857020-75-8P, 6-Benzofurancarboxylic acid, 2-ethyl- 857021-42-2P, Benzofuran, 2,7-diethyl-
RL: PREP (Preparation)
(preparation of)

IT 94302-86-0P, Ketone, 2,5-diethyl-3-benzofuranyl p-hydroxyphenyl 101894-27-3P, Benzofuran, 6-acetyl-2-ethyl-3-p-hydroxybenzoyl-
RL: PREP (Preparation)
(preparation of)

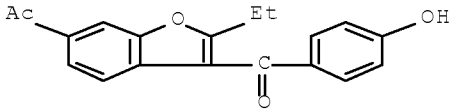
RN 94302-86-0 CAPLUS

CN Ketone, 2,5-diethyl-3-benzofuranyl p-hydroxyphenyl (6CI, 7CI) (CA INDEX NAME)



RN 101894-27-3 CAPLUS

CN Phenol, p-(6-acetyl-2-ethyl-3-benzofuranylcarbonyl)- (6CI) (CA INDEX NAME)



L27 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:569050 CAPLUS Full-text

DOCUMENT NUMBER: 143:97254

TITLE: Process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and dealkylation

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PATENT ASSIGNEE(S): Clariant France, Fr.

SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2864536	A1	20050701	FR 2003-15398	20031224
FR 2864536	B1	20060317		
WO 2005066149	A1	20050721	WO 2004-IB4158	20041215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1699772	A1	20060913	EP 2004-801395	20041215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1898226	A	20070117	CN 2004-80038285	20041215
JP 2007517012	T	20070628	JP 2006-546365	20041215
NO 2006002936	A	20060922	NO 2006-2936	20060623
IN 2006CN02324	A	20070706	IN 2006-CN2324	20060626
US 2007155831	A1	20070705	US 2006-584440	20061129
PRIORITY APPLN. INFO.:			FR 2003-15398 A	20031224
			WO 2004-IB4158 W	20041215

OTHER SOURCE(S): CASREACT 143:97254
ED Entered STN: 01 Jul 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is related to the preparation of benzofurans I [R = linear or branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5- nitrobenzofuran with SOCl2 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlCl3 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°).

IC ICM C07D307-80
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45
IT 856758-05-9P, 2-(n-Butyl)-3-(2-hydroxybenzoyl)-5-nitrobenzofuran
RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)
IT 141645-16-1P, 2-(n-Butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran

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     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (product; process for preparation de 2-(n-alkyl)-3-(4-
        hydroxybenzoyl)benzofurans and intermediates by halogenation of the
        corresponding carboxybenzofurans, Friedel-Crafts acylation with
        alkoxybenzenes and dealkylation)
REFERENCE COUNT:         5     THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


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